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Semiclassical Green functions in mixed spaces

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Abstract

A explicit formula on semiclassical Green functions in mixed position and momentum spaces is given based on Maslov's multi-dimensional semiclassical theory. The general formula includes both coordinate and momentum representations of Green functions as two special cases of the form.

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Semiclassical methods are as old as quantum mechanics and an enormous amount of work has been done in the field. Among them, the WKB method can be found in any standard quantum mechanics textbooks.[1] But it is usually confined in one dimensional case. There has long been a need for the development of a method that can be used to deal with multi-dimensional problems. In last two decades, the Maslov and Fedoriuk's (MF) n-dimensional semiclassical theory[2] has achieved a remarkable success in atomic and molecular physics field.[3] The semiclassical method emphasizes a suitable choice of representation space (usually a mixed position-momentum space) to overcome the semiclassical diversity in configuration or momentum space. Delos has shown how to construct a uniform semiclassical wave function by MF's approach.[4] The semiclassical Green functions or propagators in configuration and momentum space has been available for a long time.[5] But they can not work in the singular regions such as near caustics or foci of classical trajectories. Semiclassical Green functions and trace formulas in connection with caustics are analyzed in detail by Littlejohn and coworkers[6].[7] They emphasize geometrical properties of the semiclassical trace formula and shows the intrinsic property of Maslov index. In this paper we want to construct a semiclassical Green function explicitly in mixed position-momentum spaces, which can be used locally to fix the diversity of its counterpart in configuration or momentum space at any boundaries between classically allowed and classically forbidden regions. The Green function in mixed space is important to construct to a uniform semiclassical Green function in customary configuration space. In fact, in above mentioned singular regions we can obtain a uniform semiclassical Green function in following steps: Firstly, we transform the primitive Green function in configuration space into a suitable chosen mixed space. Then a finite Green function in the mixed space is calculated. Finally, we transform it back into configuration space, and sewing it with the primitive Green function smoothly to construct a uniform semiclassical Green function. In the following we will achieve the three steps explicitly.

For simplicity's sake we consider a single particle without spin in n-dimensional configuration space, and its Hamiltonian independent of time. The propagator at constant energy or Green function $G\left(q', q'', E\right)$ satisfies the inhomogeneous equation

$$[E - H(p'', q'')]G\left(q', q'', E\right) = \delta\left(q'' - q'\right) \tag{1}$$

where q' is the initial position, q'' the final position and E is the total energy. The semiclassical approximation $\tilde{G}$ of G is given by[5]

$$\tilde{G}(q'', q', E) = \frac{2\pi}{(2\pi i\hbar)^{(n+1)/2}} \sum_{class.\ traj.} (|D_s|)^{1/2} \exp\left[\frac{i}{\hbar}\left(S - \mu\frac{\pi}{2}\right)\right] \tag{2}$$

where

$$S(q'', q', E) = \int_{q'}^{q''} p dq, \tag{3}$$

is the classical action evaluated along the classical path which leads from q' to q'' at the given energy $H(p,q) = E$ and μ is the Maslov index, which is related with topological property of the ray of trajectories. Its geometrical properties has been discussed in detail by Littlejohn and coworkers[6].[7] The summation in Eq.(2) is over all classical trajectories from q' to q''. The determinant D_s is defined as

$$D_s = \left| \begin{array}{cc} \frac{\partial^2 S}{\partial q' \partial q''} & \frac{\partial^2 S}{\partial q' \partial E} \\ \frac{\partial^2 S}{\partial E \partial q''} & \frac{\partial^2 S}{\partial E^2} \end{array} \right|. \tag{4}$$

which is a $n+1$ th determinant and can be considerably simplified as $n-1$th one if introducing a local coordinate system centered on the trajectory[56].[7] Denote the coordinates $(\mathbf{y}, z)$, with z runs along the trajectory and $n-1$ coordinates $\mathbf{y}$ transverse to the path in such a way $y = 0$ specifies the path. In the local coordinate,

$$D_s = \frac{1}{|\dot{z}'\dot{z}''|} \left| \frac{\partial^2 S}{\partial \mathbf{y}' \partial \mathbf{y}''} \right|. \tag{5}$$

In fact, above restrictions on the local coordinate are not necessary and have been shown in Refs.(6) and (7).

The semiclassical propagator in momentum space is given , in analogy of its counterpart in configuration space, by

$$\tilde{F}(p'', p', E) = \frac{2\pi}{(2\pi i\hbar)^{(n+1)/2}} \sum_{class.\ traj.} (|D_T|)^{1/2} \exp\left[\frac{i}{\hbar}\left(T - \nu\frac{\pi}{2}\right)\right], \tag{6}$$

where

$$T(p'', p', E) = -\int_{p'}^{p''} q dp, \tag{7}$$

is the classical action along the classical path from p' to p'' at the given energy $H(p,q) = E$ and ν is the Maslov index calculated in momentum

space. Usually, $\nu \neq \mu$ because of the different topological properties of trajectories between configuration and momentum spaces. The determinant D_T is defined in an analogy way as

$$D_T = \begin{vmatrix} \frac{\partial^2 T}{\partial p' \partial p''} & \frac{\partial^2 T}{\partial p' \partial E} \\ \frac{\partial^2 T}{\partial E \partial p''} & \frac{\partial^2 T}{\partial E^2} \end{vmatrix}. \tag{8}$$

Applying a similar local coordinate in momentum space, say, p_z and $\mathbf{p}_y$ are along and transverse the trajectory respectively, we have the stability matrix in momentum space

$$D_T = \frac{1}{|\dot{p}'_z \dot{p}''_z|} \left| \frac{\partial^2 T}{\partial \mathbf{p}'_y \partial \mathbf{p}''_y} \right| \tag{9}$$

According quantum mechanics Green functions both in position and momentum spaces must be finite. However, semiclassical approximation of them contain divergences at any boundary between classically allowed and classically forbidden regions, and at any caustics or foci of classical trajectories. The reason causing such divergences is not the semiclassical theory itself, but configuration or momentum representations are not suitable in these singular regions. If we transform the problem to some mixed position-momentum representation, such divergences can be repaired. It has been shown that there "almost always" exists a representation in which the semiclassical approximation does not divergent in these singular regions[2].[4]

We choose mixed coordinates (p_α, q_β), where $\alpha = 1, \cdots, k$ and $\beta = k + 1, \cdots, n, i.e$, which are disjoints set. So the set $p_\alpha q_\beta$ contains no canonical conjugate pairs. The propagator or Green function in the mixed space can be acquired from the counterpart in configuration space by partial Fourier transformation. The propagator $F\left(p''_\alpha q''_\beta, p'_\alpha q'_\beta E\right)$ from $p'_\alpha q'_\beta$ to $p''_\alpha q''_\beta$ while propagating with the energy E, is defined by

$$\begin{aligned} F\left(p''_\alpha q''_\beta, p'_\alpha q'_\beta E\right) &= (2\pi\hbar)^{-k} \int dq''_\alpha \int dq'_\alpha G\left(q'' q' E\right) \\ &\quad \times \exp\left[i\left(p'_\alpha q'_\alpha - p''_\alpha q''_\alpha\right)/\hbar\right]. \end{aligned} \tag{10}$$

Its semiclassical approximation $\tilde{F}\left(p''_\alpha q''_\beta, p'_\alpha q'_\beta E\right)$ can be acquired by inserting $\tilde{G}\left(q'' q' E\right)$ into Eq.(10) and evaluating the integral by $k-$dimensional stationary phase approximation(SPA). Firstly, we calculate the integral on q'_α , that is

$$\tilde{F}\left(q'', p'_\alpha q'_\beta E\right) \approx (2\pi\hbar)^{-k/2} \int dq'_\alpha \tilde{G}\left(q'' q' E\right) \exp\left[i\left(p'_\alpha q'_\alpha - p''_\alpha q''_\alpha\right)/\hbar\right]. \tag{11}$$

where $\tilde{F}\left(q'', p'_\alpha q'_\beta E\right)$ represents the integral after SPA. Inserting Eq.(2) into the expression, the exponent becomes

$$\tilde{S} = S(q''q'E) + p'_\alpha q'_\alpha - p''_\alpha q''_\alpha \tag{12}$$

apart from the factor $i/\hbar$. It is noted that we adopt a single $\tilde{S}$ to denote the exponent before and after SPA. For convenience, Maslov index and the summation over classical orbits have been dropped temporarily. The SP points $q'_{\alpha 0}$ satisfy

$$\left.\frac{\partial S}{\partial q'_\alpha}\right|_{q'_{\alpha 0}} = -p'_\alpha, \quad \alpha = 1, \cdots, k. \tag{13}$$

After SPA, the preexponential factor can be written as

$$\begin{aligned} & \frac{2\pi}{(2\pi i\hbar)^{(2n+1)/2}} \cdot \frac{(2\pi i\hbar)^{k/2}}{(2\pi\hbar)^{k/2}} (D_s)^{1/2} \left(\frac{\partial^2 \tilde{S}}{\partial^2 q'_\alpha}\right)^{-1/2} \\ = & \frac{2\pi i^{k/2}}{(2\pi i\hbar)^{(2n+1)/2}} (D_s)^{1/2} \left(-\frac{\partial q'_\alpha}{\partial p'_\alpha}\right)^{1/2}. \end{aligned} \tag{14}$$

To simplify the expression further, we rewrite D_s as

$$D_s = \begin{vmatrix} \frac{\partial^2 S}{\partial q'_\alpha \partial q''_\alpha} & \frac{\partial^2 S}{\partial q'_\alpha \partial q''_\beta} & \frac{\partial^2 S}{\partial q'_\alpha \partial E} \\ \frac{\partial^2 S}{\partial q'_\beta \partial q''_\alpha} & \frac{\partial^2 S}{\partial q'_\beta \partial q''_\beta} & \frac{\partial^2 S}{\partial q'_\beta \partial E} \\ \frac{\partial^2 S}{\partial E \partial q''_\alpha} & \frac{\partial^2 S}{\partial E \partial q''_\beta} & \frac{\partial^2 S}{\partial E^2} \end{vmatrix}, \tag{15}$$

and the second derivatives of S now should be replaced the derivatives of $\tilde{S}$. To achieve the replacement, we can use the following relations

$$\begin{aligned} \frac{\partial S}{\partial q'_\alpha} &= -p'_\alpha, \\ \frac{\partial \tilde{S}}{\partial q''_\alpha} &= \frac{\partial S}{\partial q''_\alpha}, \\ \frac{\partial \tilde{S}}{\partial E} &= \frac{\partial S}{\partial E}. \end{aligned} \tag{16}$$

Inserting Eqs.(15) and (16), Eq.(14) becomes

$$
\frac{2\pi i^{k/2}}{(2\pi i\hbar)^{(2n+1)/2}} \begin{vmatrix} \frac{\partial^2 \tilde{S}}{\partial p'_\alpha \partial q''_\alpha} & \frac{\partial^2 \tilde{S}}{\partial p'_\alpha \partial q''_\beta} & \frac{\partial^2 \tilde{S}}{\partial p'_\alpha \partial E} \\ \frac{\partial^2 S}{\partial q'_\beta \partial q''_\alpha} & \frac{\partial^2 S}{\partial q'_\beta \partial q''_\beta} & \frac{\partial^2 S}{\partial q'_\beta \partial E} \\ \frac{\partial^2 S}{\partial E \partial q''_\alpha} & \frac{\partial^2 S}{\partial E \partial q''_\beta} & \frac{\partial^2 S}{\partial E^2} \end{vmatrix}^{1/2} \equiv \frac{2\pi i^{k/2}}{(2\pi i\hbar)^{(2n+1)/2}} \left(D'_{\tilde{s}}\right)^{1/2} \tag{17}
$$

It is noted that in the first line S is replaced by $\tilde{S}$. After SPA, the integral in Eq.(11) becomes

$$
\tilde{F}\left(q'', p'_\alpha q'_\beta E\right) = \frac{2\pi i^{k/2}}{(2\pi i\hbar)^{(2n+1)/2}} \left(D'_{\tilde{s}}\right)^{1/2} \exp\left(\frac{i}{\hbar}\tilde{S}\right), \tag{18}
$$

where

$$
\tilde{S} = S(q'' q'_{\alpha 0} q'_\beta E) + p'_\alpha q'_{\alpha 0} - p''_\alpha q''_\alpha. \tag{19}
$$

is the value of Eq.(12) at the first SP point. Secondly, we again approximate the integral over q''_α by SPA to get the mixed Green function

$$
\tilde{F}\left(p''_\alpha q''_\beta, p'_\alpha q'_\beta E\right) \approx (2\pi\hbar)^{-k/2} \int dq''_\alpha \tilde{F}\left(q'', p'_\alpha q'_\beta E\right). \tag{20}
$$

Again $\tilde{F}\left(p''_\alpha q''_\beta, p'_\alpha q'_\beta E\right)$ denotes the integral after SPA. The SP points now satisfy

$$
\left.\frac{\partial S}{\partial q''_\alpha}\right|_{q''_{\alpha 0}} = -p''_\alpha, \quad \alpha = 1, \cdots, k. \tag{21}
$$

The relations in Eq.(16) are replaced by

$$
\begin{aligned}
\frac{\partial S}{\partial q''_\alpha} &= -p''_\alpha, \\
\frac{\partial \tilde{S}}{\partial q'_\beta} &= \frac{\partial S}{\partial q'_\beta}, \\
\frac{\partial \tilde{S}}{\partial q''_\beta} &= \frac{\partial S}{\partial q''_\beta}, \\
\frac{\partial \tilde{S}}{\partial E} &= \frac{\partial S}{\partial E},
\end{aligned} \tag{22}
$$

which leads to the replacement of the derivatives with respect to q''_α in the first column of $D'_{\tilde{S}}$ by the ones to p''_α. Then the preexponential factor arrives at

$$\frac{2\pi i^{k/2}}{(2\pi i\hbar)^{(2n+1)/2}}\begin{vmatrix} \frac{\partial^2\tilde{S}}{\partial p'_\alpha\partial p''_\alpha} & \frac{\partial^2\tilde{S}}{\partial p'_\alpha\partial q''_\beta} & \frac{\partial^2\tilde{S}}{\partial p'_\alpha\partial E} \\ \frac{\partial^2\tilde{S}}{\partial q'_\beta\partial p''_\alpha} & \frac{\partial^2\tilde{S}}{\partial q'_\beta\partial q''_\beta} & \frac{\partial^2\tilde{S}}{\partial q'_\beta\partial E} \\ \frac{\partial^2\tilde{S}}{\partial E\partial p''_\alpha} & \frac{\partial^2\tilde{S}}{\partial E\partial q''_\beta} & \frac{\partial^2\tilde{S}}{\partial E^2} \end{vmatrix}^{1/2} \equiv \frac{2\pi}{(2\pi i\hbar)^{(2n+1)/2}}\left(D_{\tilde{s}}\right)^{1/2} \qquad (23)$$

It is noted that the factor i^k after two integrations has been absorbed in the final determinant $D_{\tilde{S}}$. Therefore, the final Green function in $p_\alpha q_\beta$ space is

$$\tilde{F}\left(p''_\alpha q''_\beta, p'_\alpha q'_\beta E\right) = \frac{2\pi}{(2\pi i\hbar)^{(2n+1)/2}}\sum_{class.\ traj.}\left(|D_{\tilde{S}}|\right)^{1/2}\exp\left[\frac{i}{\hbar}\left(\tilde{S}-\tilde{\nu}\frac{\pi}{2}\right)\right], \qquad (24)$$

where

$$\tilde{S} = S(q''_{\alpha 0}q''_\beta q'_{\alpha 0}q'_\beta E) + p'_\alpha q'_{\alpha 0} - p''_\alpha q''_{\alpha 0}. \qquad (25)$$

is the value of Eq.(12) at the second SP point though with the same symbol. In Eq.(24) the Maslov index $\tilde{\nu}$ has been added and is related with the topological properties of classical trajectories in the mixed space. The summation over classical trajectories has also been attached. For convenience we have adopted the single symbol $\tilde{S}$ to represent the phase factor before and after SPA. $\tilde{S}$ can be written in a regular form

$$\tilde{S} = \int_{q'_\beta}^{q''_\beta} p_\beta dq_\beta - \int_{p'_\alpha}^{p''_\alpha} q_\alpha dp_\alpha \qquad (26)$$

which is the classical action evaluated the trajectory from $p'_\alpha q'_\beta$ to $p''_\alpha q''_\beta$ at given energy $H(pq) = E$. It can be acquired by differentiate Eq.(25) with respect to the terminal coordinates. Eq.(25) can be rewritten as

$$\tilde{S} = \int_{q'_{\alpha 0}}^{q''_{\alpha 0}} p_\alpha dq_\alpha + \int_{q'_\beta}^{q''_\beta} p_\beta dq_\beta + p'_\alpha q'_{\alpha 0} - p''_\alpha q''_{\alpha 0}. \qquad (27)$$

which has contained the first term in Eq.(26). Differentiating it with respect to p'_α , we have

$$\frac{\partial\tilde{S}}{\partial p'_\alpha} = -p'_\alpha\frac{\partial q'_{\alpha 0}}{\partial p'_\alpha} + q'_{\alpha 0} + p'_\alpha\frac{\partial q'_{\alpha 0}}{\partial p'_\alpha} = q'_{\alpha 0}\left(p'_\alpha\right). \qquad (28)$$

Similarly, one finds that

$$\frac{\partial\tilde{S}}{\partial p''_\alpha} = -q''_{\alpha 0}\left(p''_\alpha\right). \qquad (29)$$

Eq.(28) and (29) immediately leads to (26).

The stability matrix $D_{\tilde{s}}$ can also be simplified as a $n-1$th determinant depending on the choice of local coordinate centered on the trajectory in the mixed space. If we choose a position coordinate z along with the trajectory in the mixed space, $(p_\alpha, \mathbf{y}_\beta)$ transverse the path, then

$$D_{\tilde{S}} = \frac{1}{|\dot{z}'\dot{z}''|} \begin{vmatrix} \frac{\partial^2 \tilde{S}}{\partial p'_\alpha \partial p''_\alpha} & \frac{\partial^2 \tilde{S}}{\partial p'_\alpha \partial \mathbf{y}''_\beta} \\ \frac{\partial^2 \tilde{S}}{\partial \mathbf{y}'_\beta \partial p''_\alpha} & \frac{\partial^2 \tilde{S}}{\partial \mathbf{y}'_\beta \partial y''_\beta} \end{vmatrix} . \tag{30}$$

Conversely, choosing a momentum coordinate p_z along with the trajectory and $(p_{y\alpha}, q_\beta)$ transverse the path, we have

$$D_{\tilde{S}} = \frac{1}{|\dot{p}'_z\dot{p}''_z|} \begin{vmatrix} \frac{\partial^2 \tilde{S}}{\partial p'_{y\alpha} \partial p''_{y\alpha}} & \frac{\partial^2 \tilde{S}}{\partial p'_{y\alpha} \partial q''_\beta} \\ \frac{\partial^2 \tilde{S}}{\partial q'_\beta \partial p''_{y\alpha}} & \frac{\partial^2 \tilde{S}}{\partial q'_\beta \partial q''_\beta} \end{vmatrix}$$

Formula(24) is a unified expression. If $\alpha = 0, \beta = 1 \cdots n$, it will recover as Eq.(2), the Green function in configuration space. Conversely, if $\alpha = 1 \cdots n$, $\beta = 0$, Eq.(6), the propagator in momentum space will immediately emerge.

For most semiclassical physical problems, it is convenient to work in configuration space. Eq.(2) usually works quite will in most regions. But in some regions, such as near caustics and foci of classical trajectories, it will be divergent. In these regions, we can " almost always"[24]choose a suitable set of mixed position-momentum coordinates to calculate the mixed Green function, which is not divergent. From the function, an accurate configuration-space Green function can be constructed be inverse partial Fourier transformation,

$$\begin{aligned} \tilde{G}\left(q''q'E\right) &= \left(2\pi\hbar\right)^{-k} \int dp''_\alpha \int dp'_\alpha \tilde{F}\left(p''_\alpha q''_\beta, p'_\alpha q'_\beta E\right) \\ &\quad \times \exp\left[i\left(-p'_\alpha q'_\alpha + p''_\alpha q''_\alpha\right)/\hbar\right]. \end{aligned} \tag{31}$$

Then we can sew it with the primitive Green function smoothly to get a uniform Green function.

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References

[1]For example, A. Messiah, *Quantum Mechanics*, Vol. I. North-Holland, Amsterdam, 1964, pp222-228. L. D. Landau and E. M. Lifschitz, *Quantum Mechanics*, 2nd ed. Pergamon Press, New York, 1965, p158.

[2]V. P. Maslov and M. V. Fedoriuk, *Semiclassical Approximation in Quantum Mechanics*. D. Reidel, Boston, 1981.

[3]M. L. Du and J. B. Delos, Phys. Rev. A. **38**,1896(1988); **38**,1913(1988).

[4]J. B. Delos, Adv. Chem. Phys. **65**, 161(1986).

[5]M. C. Gutzwiller, J. Math. Phys, **8**, 1979(1967); **10**, 1004(1969); **11**, 1791(1970); **12**, 343(1971); *Chaos in Classical and Quantum Mechanics*, Springer-Verlag, New York,1990.

[6]S. C. Creagh, J. M. Robbins and R. G. Littlejohn, Phys. Rev. A. **42**, 1907(1990).

[7]R. G. Littlejohn, J. Math. Phys. **31**, 2952(1990).